<Bioinformatics Center> Bioknowledge Systems

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- Bioknowledge Systems -

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Scope of Research

Owing to continuous developments of high throughput experimental technologies, projects are going on not only to determine complete genome sequences of an increasing number of organisms, but also to analyze gene expression profiles both at the mRNA and protein levels and to catalog protein 3D structure families. Bioinformatics provides basic concepts as well as practical methods to go up from the molecular level to the cellular level, and eventually to still higher levels, to that of biological systems by analyzing complex interactions among building blocks and with dynamic environments. We have been developing such bioinformatics technologies and the KEGG system (http://www.genome.jp/kegg/), which is our attempt to uncover and utilize cellular functions through the reconstruction of protein interaction networks from genome information.

Research Activities (Year 2005)

Grants

Kanehisa M, Education and Research Organization for Genome Information Science, MEXT.

Kanehisa M, BRITE: Deductive Database of the Genome and the Biological System Based on Binary Relations, Bioinformatics Research and Development, JST.

RPAIR: a Database of Chemical Transformation Patterns in Enzymatic Reactions

Chemical genomics is the next stage of post-genomic analysis. Drugs, environmental substances and various chemical compounds contribute to the fluctuation of bio-systems. Therefore, chemical genomic analysis would require the investigation of relationships between genomes and their extracellular environments.

These relationships between bio-systems and environments include complicated biochemical reactions. At present, biochemical reactions are hierarchically classified using EC (Enzyme Commission) numbers. However, the classification is not totally based on chemical reactions, but also include enzymes or enzyme genes. EC numbers are commonly utilized as identifiers of enzymes or enzyme genes.

In order to expand our current limited knowledge on biochemical reactions as represented by EC numbers, we developed a novel database that provides the patterns of the conformational changes between the chemical structures of the substrate and product. This database is integrated into the KEGG resource, so other databases in KEGG have links to the entries of this database. All of the data is available from http://www.genome.jp/reaction/.

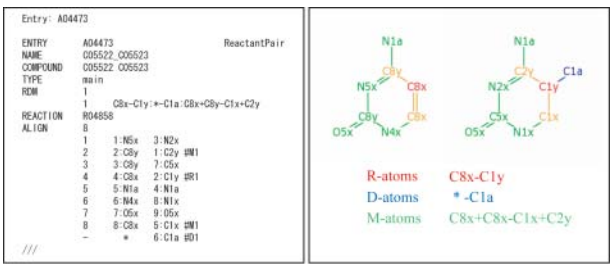

Figure 1. An RPAIR database entry (left) and the assignment of R-, D- and M- atoms (right).

KAAS : an Automatic Functional Annotation Server for New Genomes

KEGG Orthology (KO), which is developed from the "Ortholog ID", an extension of the EC number in the KEGG PATHWAY database, is one of our major projects and is intended to identify and classify orthologous gene clusters among all species computationally and manually.

Recently, a number of draft- and completely - sequenced genomes are rapidly growing. Therefore, we need a speedy and easy method to annotate gene functions. KEGG Automatic Annotation Server (KAAS), which is a web-based server, provides functional annotation of genes by BLAST comparisons against the manually curated KEGG GENES database and a heuristic method. The result contains hierarchical KO assignments and automatically generated KEGG pathways. We have been using this method effectively to annotate draft genomes and EST clusters, which we provide as the DGENES and EGENES databases.

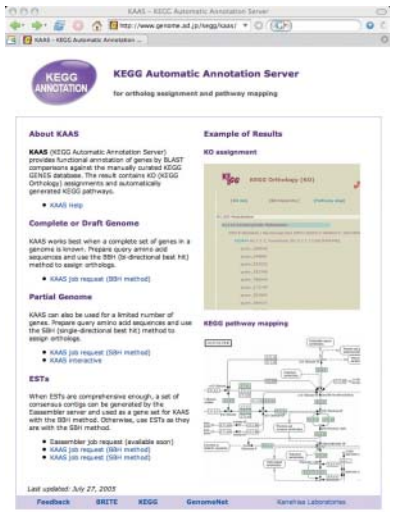

Figure 2. KAAS: KEGG Automatic Annotation Server (http://www.genome.jp/kegg/kaas/).

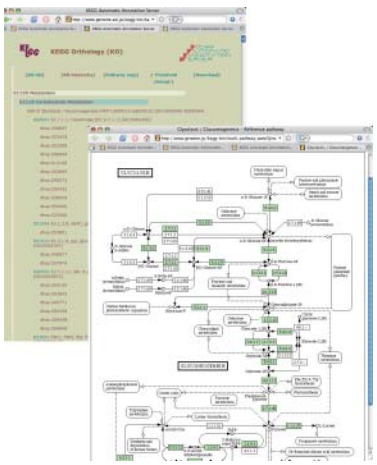

Figure 3. Results of KAAS. KO assignment (left) and generated pathway (right).

Kanehisa M, Center of Research and Knowledge Information Infrastructure for Genome Science. Kyoto University 21st Century COE Program, MEXT.

Kanehisa M, Biological Systems Database, Grants-in-Aid for Scientific Research on Priority Areas, MEXT.

Kanehisa M, Bioinformatics Training Unit; Education and Research Organization for Genome Information Science. MEXT.

Goto S, Probing the *Plasmodium falciparum* Genome, Contact Research, JST.